Chapter 3: Nuclear and Atomic Data

Introduction

In order to transport neutrons and photons TART95 requires nuclear and atomic data to describe the interaction of neutrons with nuclei and photons with atoms. It also need data to describe neutron induced photon production, which can also be transported.

Sources of Data

The standard source of data used by TART95 is the Livermore ENDL [9], neutron interaction and neutron induced photon production data, and EGDL, photon interaction data. Additional, non-standard neutron interaction data based on ENDF/B-VI is also available. The ENDF/B-VI photon interaction library is based on the Livermore EGDL data, so that it isn't necessary to have an alternative library.

The ENDL neutron interaction data is at room temperature (293 Kelvin) and is processed into the form used by TART95, i.e., 175 group constants. See, the appendix for a table of the TART95 neutron 175 energy group boundaries. Additional, non-standard, neutron interaction data files are also available, based on data from other libraries, as well as at other temperatures; using the SIGMA1 method of Doppler broadening [31, 36] data can be prepared at any temperature. One available alternative library is based on what we feel is an optimum combination of ENDF/B-VI cross sections (which are good at lower energies) and ENDL kinematics (which are good at higher energies). In order to create libraries at other temperatures, rather than processing an entire data library (cross sections, angular distribution, energy distributions, etc.) for most applications it is adequate to Doppler broaden only the total, elastic, capture and fission cross sections using program GROUPIE [31] and then use program GROUPIE [31] to create multi-band parameters for direct use in TART95.

The EGDL photon interaction data is the original source of the ENDF/B-VI library [14]. For use in TART95 the EGDL cross sections are processed into a fixed energy grid of 176 energy points between 100 eV and 30 MeV. The same fixed energy grid is used for all materials. This 176 energy point grid is dense enough to allow linear interpolation between adjacent tabulated data points. See the appendix for a table of the TART95 photon 176 energy points. The use of a fixed energy grid for all materials and linear interpolation significantly reduces running time and yet allows a representation of the data to well within its uncertainty.

The ENDL neutron induced photon production data is currently the only source of this type of data available to TART95. In TART95 neutron induced photon production is completely uncorrelated to the individual neutron interactions that occur. This may sound strange at first, but as actually used it significantly reduces running time and better simulates what is actually measured and reported in neutron induced photon production measurements. For example, in such measurements what is measured and best known is

the total production of photons from all competing processes, not the production from each and every process.

WARNING - The ENDL neutron interaction and neutron induced photon production cross sections have been designed to be completely consistent when used in combination, as have other neutron data libraries. But the user MUST be aware that to perform consistent coupled neutron-photon transport calculations if you use any alternative data sets you MUST consistently use both neutron interaction and photon production data from the same alternative set of data. For example, for coupled neutron-photon calculations you SHOULD NOT use ENDF/B-VI neutron interaction data and ENDL neutron induced photon production data. If you are only performing neutron (not photon) transport calculations you can use any of the available neutron data files.

Use of Data by TART95

TART95 uses continuous energy neutrons and photons. However, to represent the neutron cross sections it uses multigroup cross sections. For example, when tracking neutrons if the neutron energy is within the energy limits of a given energy group the cross sections for that group are used to define how far the neutron will transport between collisions (based on the total cross section), as well as what type of collision occurred (based on the individual cross sections for elastic, capture, fission, etc.). When the collision occurs starting from the original neutron energy the neutron can be scattered or transferred to any other energy based on the kinematics of the type of collision. Even though the neutron cross sections are in multi-group form, the scatter or transfer of neutrons between energies is done on a continuos energy basis. Neutrons are not constrained in any way to have discrete energies based on the energies of the multigroup cross sections; neutron energies are continuous and can have any value between the maximum and minimum allowed energies.

Expected Energy Deposition

In order to allow TART95 to perform expectation, as well as analog, calculations. TART95 uses expected energy depositions which have been pre-calculated from the ENDL and EGDL data [9, 14] and is included in the TART95 neutron interaction data file TARTND and photon interaction file GAMDAT. Based on the kinematics of each process expected energy deposition is pre-calculated for both neutron and photon interactions. Energy deposition is included separately for each process, e.g., there are separate energy deposition tables for elastic, inelastic, fission, etc. The details of how energy deposition is calculated are included in the documentation for the processing system OMEGA [8] and will not be discussed in detail here. Here we will only include sufficient detail to allow users to understand the physical significance of the data used.

In order to allow TART95 to track either only neutrons or neutrons and photons the TART95 data file for neutron interactions, TARTND, contains two sets of expected energy deposition.

For use when only tracking neutrons, one set of deposition is defined as the energy of all secondary particles EXCEPT neutrons. This includes the energy of all photons, charged particles, recoil nucleus, fission products, etc.

For use when tracking neutrons and photons, one set of deposition is defined as the energy of all secondary particles EXCEPT neutrons and photons. This includes the energy of all charged particles, recoil nucleus, fission products, etc.

The file for photon interactions, GAMDAT, has only one set of energy deposition for each process. For coherent scattering there is no energy loss and therefore the deposition is zero. For incoherent scattering deposition is based on the integral of the product of the Klein-Nishina formula and the incoherent scattering function. For pair production the energy deposition is defined as the incident energy of the photon minus 1.022 MeV (the rest mass equivalent of the two 0.511 MeV photons produced when the positron annihilates). For photoelectric the table in GAMDAT is the incident photon energy minus the energy of all fluorescence x-rays. The default option for TART95 is not to track fluorescence x-rays, so that if the track fluorescence option (**sentl 25**) is not used fluorescence x-rays will not be tracked and internally TART95 redefines the photoelectric energy deposit to be the energy of the incident photon.

Based on the TART95 input options specified for each problem that affect expected energy deposition, e.g., track or don't track photons, track or don't track fluorescence x-rays, TART95 selects the appropriate energy depositions for each process. These are then combined with the cross sections for the problem to define the macroscopic total energy deposition in MeV/cm for each material in the problem. During particle tracking TART95 uses these macroscopic total energy depositions in combination with particle track lengths between collisions to estimate expected energy deposition.

Multi-Group vs. Multi-Band Cross Sections

For neutron transport TART95 uses 175 multi-group cross sections; see table 1 in the appendix for a list of the energy boundaries of the 175 groups. When generating multi-group cross sections we must assume some approximation for the energy dependent flux, or weighting, within each group. Usually this will involves the product of two terms: an energy dependent spectrum, e.g., Maxwellian, 1/E, fission, fusion spectra at successively higher energies, and a self-shielding factor, e.g., $1/sig_{tot}$.

Using 175 groups, all of which are fairly narrow, the results are fairly insensitive to the energy dependent spectrum used. For use with TART95 the standard libraries include a "flat", or constant, spectrum, and a second library using a Maxwellian, 1/E, fission, fusion spectrum at successively higher energies.

In normal multi-group calculations selecting one general purpose self-shielding factor to use in general purpose libraries, such as those used by TART95, is a difficult problem.

Depending on the choice we can try to conserve reaction rates, by using "no", or a unity self-shielding factor, or distance to collision, by using $1/sig_{tot}$, which is proportional to the distance to collision in a pure material, or we could use $1/[sig_{tot} + sig_0]$, which is the Bonderenko approximation to the distance to collision in a mixture of materials (here sig_0 approximates the contribution of all "other" materials in the mixture). In the case of TARTNP, which was originally designed for high energy applications where self-shielding is not as important an effect as at lower energies, it was decided that the standard multi-group library would be unshielded, i.e., the multi-group constants are simple integrals of the cross section averaged over each group and self-shielding effects are ignored. In order to extend TARTNP for use in lower energy applications the multi-band method is used to handle self-shielding effects.

In the multi-band approach [26-31] we can dynamically account for self-shielding effects in calculations. Unlike the multi-group method where we can only try to conserve one quantity of interest, e.g., reactions or distance to collision (but not both), in the multi-band approach we can simultaneously conserve a number of quantities of interest. We are not going to go into detail here, see [31], but basically rather than use one total cross section in each group, the multi-band method uses several totals in each group where each total represents the effect of different total cross section ranges. As such the approach is similar to the Probability Table Method [31], which also divides the overall variation of the total cross section in some energy range into a number of total cross section ranges. However, the multi-band method is different in the sense that while the Probability Table Method doesn't explicitly conserve anything the multi-band method directly conserves simultaneously reaction rates and distance to collision. It also differs in that the Probability Table Method is only used in the unresolved resonance region, whereas the multi-band method is used at all energies. As such the multi-band method is much more directly related to the Subgroup Method [31], which also directly conserves quantities and can be used at all energies. The multi-band method differs from the Subgroup Method mostly in terms of what quantities are conserved and how it is applied in Monte Carlo calculations. The Subgroup Method has a problem in maintaining the correlation between the cross sections for the same material in different zones that a neutron may pass through during transport, which can lead to an unreasonable number of equations that have to be solved. In the multi-band method this problem is completely avoided by, after each event, sampling cross sections for all the materials in the problem, and consistently using only these sampled cross sections to transport the neutron through any number of zones until the next event occurs; thereby exactly correlating the cross sections for the same material in all zones (again, for details see [31]).

In analog Monte Carlo calculations using multi-group cross sections our basic problem is how to transport from one space point A where a neutron has had a collision to the next space point B where it will have its next collision. In terms of considering results integrated over some energy range (one of the groups) this problem is completely analogous to the problem of calculating the uncollided transmission through a material starting from neutrons distributed within a given energy range. If each experimental energy range corresponds to one of the multi-groups normal multi-group calculations would

predict that the neutrons will be exponentially attenuated through the material (we would obtain a straight line result on a semi-log plot of distance through the material versus uncollided transmission). In fact experiment results using materials that have resonance structure show a typical self-shielding curve, with a rapid decrease in uncollided transmission for small material thicknesses, and a slower decrease for thicker materials. This merely indicates that for small material thicknesses the neutrons interact with the high cross sections near the peaks of the resonances and are rapidly attenuated. For larger thicknesses all of the neutrons that were near the peaks of the resonances have been removed and only those neutrons interacting with smaller cross sections between the resonances remain and these are attenuated much more slowly as the material thickness increases.

The most important point to understand is that the self-shielding curves that result from experiments indicate that a single multi-group cross section cannot be used to reproduce these results. It doesn't matter whether you use shielded or unshielded cross sections; one single cross section cannot reproduce a self-shielding curve. A single multi-group cross section predicts simple exponential attenuation based on this constant cross section. With unshielded or shielded cross sections you will have different exponential attenuation, but in each case you will have simple exponential attenuation. In contrast, the self-shielding curves indicate that the effective multi-group cross section is decreasing as the neutrons transport further and further into the material. What the multi-band method does is simulate these self-shielding curves by using more than one total cross section in each group. Although experimentally measured self-shielding curves cannot be produced using only one cross section that results in simple exponential attenuation, it can be reproduced using several different cross sections each of which will result in a different simple exponential attenuation, but the sum of which agrees with measured self-shielding curves. When averaged over the sum of exponentials to define an equivalent single multi-group cross section the multi-band approach is equivalent to using a continuously and smoothly varying total cross section as a function of the distance transported by the neutrons, which is what we want to simulate experimental measurements, or more to the point as it applies to TART95, simply going from point A to point B between collisions in the Monte Carlo calculation.

Basically the multi-band method uses the analytical results of certain limiting transport situations to guarantee that when we encounter these limiting situations our solution reduces to the correct limit. Fortunately there aren't that many limiting situations that we have to worry about (once described as meaning that "Nature is user friendly") and we can end up with multi-band cross sections that can be used in general. What limiting cases should we consider? For cases where a material is optically thin (thin in terms of mean free paths) what a distribution of neutrons over an energy interval will interact with is the unshielded cross section (just in terms of cause and effect, at the point where neutrons are incident on a material or have not yet transported any distance, they haven't "seen" the material yet, so that the flux cannot be self-shielded). For optically thick material the cross section that the neutrons "see" when averaged over its path length through many mean free paths corresponds to the $1/sig_{tot}$ weighted cross section, or equivalently averaged

using the distance to collision as a weighting factor. Similarly if we consider the results of transport theory, in optically thick media the narrow resonance approximation predicts that $1/sig_{tot}$ weighting should be used; yet another limiting case to consider. Other intermediate cases can be based on the narrow resonance approximation where the Bonderenko self-shielding model predicts a weighting of $1/[sig_{tot} + sig_0]$, where sig_{tot} is the cross section of one material and sig_0 is an energy independent approximation used to represent the effect of other materials in a mixture. Sig_0 can vary from infinity, which reproduces unshielded results, to zero, which produces totally shielded $1/sig_{tot}$ weighted results. Note, although uncollided transmission measurements and the narrow resonance and Bonderenko approximations correspond to completely different physical situations, both predict fluxes with a self-shielded form $1/[sig_{tot} + sig_0]$. Therefore if we can produce fluxes of this form we can simultaneously conserve all of these cases and force our Monte Carlo to rapidly converge to the correct limits.

The multi-band method assumes that we have pre-calculated multi-group cross sections using a number of different self-shielding models. Starting from these pre-calculated results it then defines multi-band parameters to exactly conserve these pre-calculated results, that when used in applications will exactly reproduce a set of limiting cases. For example, program GROUPIE [34] can be used to calculate unshielded cross sections, and self-shielded cross sections for 23 values of sig_0 using the Bonderenko $1/[sig_{tot} + sig_0]$ weighting, as well as results using $[1/sig_{tot}]^2$ and $[1/sig_{tot}]^3$ weighting. In order to physically understand the significance of this weighting by higher powers of the reciprocal of the total cross section, remember that $1/sig_{tot}$ is proportional to the distance to collision, so that reciprocal weighting by higher reciprocal powers of the total cross section is equivalent to weighting by powers of the distance to collision. For example, if we choose to conserve the results using $1/sig_{tot}$ and $[1/sig_{tot}]^2$ weighting, this is equivalent to conserving the first two moments of the distance to collision, which obviously conserves the distance to collision, but used in combination these two moments will also conserve the variance of the distribution of distances to collision.

One possible approach is to conserve the unshielded, $1/sig_{tot}$, and $[1/sig_{tot}]^2$, weighted cross sections. The option in GROUPIE [34] is still available to conserve these three moments of the cross section (using 0, 1, and 2, reciprocal powers of the total cross section as weighting). However, experience over the last twenty years indicates that a much better approach is to conserve the 0 and 1 reciprocal powers of the total cross section, but rather than conserving the $[1/sig_{tot}]^2$ weighted cross sections, we conserve the cross sections using a weight of $1/[sig_{tot} + sig_0]$, where sig_0 is defined to be the unshielded total average cross section in each group for each material. Compared to conserving the $[1/sig_{tot}]^2$ weighted cross sections, conserving the $1/[sig_{tot} + sig_0]$ weighted cross sections produces much better results when mixtures of materials are used in problems. This is the GROUPIE [34] option that has now been used for many years to produce the multi-band parameters used by TARTNP.

For the details of the following see [31]. Consider the case where we have pre-calculated multi-group cross sections using three different self-shielding weights: $<sig_0>$, using no

cross sections weighting, $<sig_1>$, using a cross section weight $1/sig_{tot}$, and $<sig_2>$, using $1/[sig_{tot} + sig_0]$, for some value of sig_0. In general the multi-band method replaces the integral over a group by a quadrature, a sum of contributions from each cross section range. So that the standard definition of a group averaged cross section,

$<sig_{tot}>$ = Reactions/Flux

is reduced to the quadrature,

$$= \text{sum}[i = 1 \text{ to } N]\ Flux_i\ sig_{toti} \,/\, \text{sum}[i = 1 \text{ to } N]\ Flux_i$$

Where the flux in each cross section band is a product of the probability of the cross section occurring, P_i, and a self-shielding factor, e.g., constant, $1/sig_{toti}$, etc.,

$$<sig_{tot}> = \text{sum}[i = 1 \text{ to } N]\ P_i\ SSF_i\ sig_{toti} \,/\, \text{sum}[i = 1 \text{ to } N]\ P_i\ SSF_i$$

where SSF_i is the self-shielding factor for band i. We assume that we have pre-calculated multi-group cross sections using a variety of self-shielding factors, so that we know $<sig_{tot}>$ and the form of SSF_i (the assumed self-shielding factor), and we solve the equations for the unknown cross section probability, P_i, and band cross section, sig_{toti}. The three forms that we assume for the self-shielding factor are,

SSF_i = 1
= $1/sig_{tot}$
= $1/(sig_{tot} + sig_0)$

and we will define sig_0 to be equal to the unshielded cross section in each group, for each material.

We can conserve all three of these moments using only two cross section bands. Each band will have a cross section probability, or weight, and a cross sections. Therefore, for two bands we have four free parameters: two probabilities and two cross sections. Since the cross section must have some value the sum of the probabilities must be unity. Therefore substituting the assumed form for the self-shielding factor, SSF_i, in the above equation, our four equations in four unknowns are,

1 = $P_1 + P_2$ (the sum of the probabilities)
$<sig_0>$ = $P_1\ sig_1 + P_2\ sig_2$ (the unshielded total cross section)
$<sig_1>$ = $1/[P_1/sig_1 + P_2/sig_2]$ ($1/sig_{tot}$ weighted)

$$<sig_2> = \frac{[P_1\ sig1/(sig_1 + sig_{0)} + P_2\ sig_2/(sig_2 + sig_{0)}]}{[P_{1/}(sig_1 + sig_{0)} + P_2/(sig_2 + sig_0)]} \quad (1/(sig_{tot} + sig_0) \text{ weight})$$

These four simultaneous equations are solved analytically (see [31]) to define the two band parameters: P_1, sig_1, P_2, and sig_2, and these parameters are used in TART95.

Following each collision that a neutron undergoes for each material in a problem the cross sections that the neutron will "see" in transporting to its next collision site are sampled from the multi-band parameters in accordance with the probability of each of the cross sections bands, i.e., select band one with probability P_1 and band two with probability P_2. It's as simple as that.

Why does this work? All we are doing is insuring that in optically thin media, where the flux is unshielded, our calculated multi-band flux will also be unshielded and we will conserve (re-produce) the correct unshielded cross section. Similarly in thick media we insure that our multi-band flux is $1/sig_{tot}$ weighted and we conserve the $1/sig_{tot}$ weighted cross section, or distance to collision. At the same time when we have a large amount of pure material the cross section will self-shield by $1/sig_{tot}$, and in a mixture by $1/[sig_{tot} + sig_0]$, and in the infinitely dilute limit there will be no self-shielding. For example, consider the analog Monte Carlo equivalent to an uncollided transmission measurement. In this case, for any thicknesses of material, X, each of the two bands will be exponentially attenuated through the material, and starting from a sampled flux in each of the two bands of P_1 and P_2, respectively, we have,

Flux $= P_1 \, Exp(-sig_{tot1} \, X) + P_2 \, Exp(-sig_{tot2} \, X)$

Reactions $= P_1 \, sig_{tot1} \, Exp(-sig_{tot1} \, X) + P_2 \, sig_{tot2} \, Exp(-sig_{tot2} \, X)$

<sig(X)> = Reactions/ Flux = equivalent multi-group cross section

Based on the standard definition of a group averaged cross section as the ratio of reactions to flux, starting from only two constant multi-bands, we obtain a continuously varying spatially dependent equivalent multi-group cross section.

Note, that at X = 0, all of the exponentials are unity, and our two band equations reduce to,

Flux $= P_1 + P_2 = 1$

Reactions $= P_1 \, sig_{tot1} + P_2 \, sig_{tot2}$

<sig(0)> = Reactions/Flux $= P_1 \, sig_{tot1} + P_2 \, sig_{tot2}$

which is exactly one of the equations we used to define the two band parameters to conserve the unshielded cross section, so that we obtain exactly the right answer in this limit.

In the other extreme of a thick medium, if we integrate over the path length, the integral of each exponential, $Exp(-sig_{toti} \, X)$ is just $1/sig_{toti}$, and the path length averages are,

Flux $= P_1 / sig_{tot1} + P_2 / sig_{tot2}$

Reactions $= P_1 \, sig_{tot1} / sig_{tot1} + P_2 \, sig_{tot2} / sig_{tot2} = P_1 + P_2 = 1$

$\langle sig(X) \rangle$ = Reactions/ Flux = $1/[P_1 / sig_{tot1} + P_2 / sig_{tot2}]$

which is exactly one of the equations we used to define the two band parameters to conserve the shielded cross section or distance to collision, so that we obtain exactly the right answer in this limit.

Conserving the additional moment using a self-shielding factor $1/[sig_{tot} + sig_0]$, where sig_0 is equal to the unshielded cross section, will force agreement with the self-shielding for a thickness, X, of about one mean free path. The net effect of conserving these three moments is to force agreement between the experimentally measured self-shielding curve and a two band analog Monte Carlo calculation.

That's the analogy to an uncollided transmission measurement. As it applies to an analog Monte Carlo calculation and the problem of transporting a neutron from point A, where it has had one collision, to point B, where it will have its next collision, this means that the sum of two bands will force the neutrons to interact according to the unshielded cross section near point A, and as the neutron transports further the effective equivalent multi-group cross section will decrease such that the average distance to collision is conserved, as will the value about one mean free path from A. Again, the overall effect is to produce the correct effective, equivalent multi-group cross section that is spatially dependent.

Later in an example criticality problem involving mixtures of uranium and water in various atom ratios we will see that the effect of conserving these moments produces the expected narrow resonance and Bonderenko approximation effects. When we have large ratios of water to uranium we produce the expected unshielded results and when we have small ratios we produce the expected self-shielded results.

TART95 uses two band cross sections over the entire energy range. Why only two bands? When the method was initially implemented in TARTNP some twenty years ago we tried up to five bands. After extensive testing the conclusion was that we couldn't see any integral effects using more than two bands. Still wouldn't it be better to use more bands anyway? We must remember that we are using the narrow resonance and Bonderenko APPROXIMATIONS - these are only approximations and using more bands would only yield results that better approximate an APPROXIMATION, not necessarily reality. Our earlier extensive testing indicated that it wasn't worth it to use more than two bands and that's all that TARTNP has used ever since then.

What about the validity of using the narrow resonance approximation over the entire energy range; what about the wide resonances that are considered in reactor theory? In general yes, this would be invalid, however with the 175 groups used by TART95 this isn't a problem, since wide resonances are resolved into different groups, so that we do not end up averaging over them and having them disappear within individual groups. **Warning** - while this works with the 175 groups used by TART95, this is not generally true for codes

that use a small number of groups. For a small number of groups the wide resonance effects should be included, which can be done using the multi-band method [28].

The user might ask: Why does TART95 use multi-group cross sections and multi-band parameters? Everybody else seems to be using continuous energy cross sections. Isn't this better? Won't continuous energy cross sections give better answers? The answer is, yes, continuous energy cross sections will give better answers, if you run your calculations forever, e.g., when your calculation involves materials that have strong, narrow resonances you have to run many, many samples to reach convergence to the correct expected average cross sections. If you want the answers accurately and fast the TART95 approach is more practical and more efficient to use.

If you want to compare the two approaches consider a material like U^{238}, that has many very narrow resonances. Let's use ENDF/B-VI data and consider a fairly narrow energy range corresponding to only one of TART95's groups from 5.763 to 7.527 keV. In this range the U^{238} capture cross section has many narrow resonances and varies over about three to four orders of magnitude. We can first use GROUPIE [34] to define the average capture cross section for this energy interval. We can then see what a Monte Carlo code using continuous energy cross sections would do to simulate transport. Randomly select an energy in this range and record the capture cross section sampled. Keep sampling and dividing by the number of samples to define an averaged sampled capture cross section. By comparing the results to the correct average defined by GROUPIE you will find that you need to sample thousands, if not hundreds of thousands of times, to obtain even a decent approximation of the correct average capture cross section. In contrast, using simple two band parameters, statistically after only two samples we will have the correct average capture cross section. That's why TART95 calculations converge so much faster.

Potentially, using continuous energy cross sections is better than using multi-groups and multi-band parameters, since this starts closer to the original evaluated data without introducing any approximations. But in most applications the results simply aren't that sensitive to what happens in one of many resonances, and it becomes too expensive to calculate long enough to insure convergence to the correct equivalent cross section averaged over many resonances (note, with all the fancy checks for convergence that Monte Carlo codes do, to our knowledge nobody ever checks for convergence to the correct, expected average cross sections). Using continuous energy cross sections is very nice and potentially more accurate, but it completely ignores everything that we know from reactor theory about the limiting values when self-shielding is involved. In contrast TART95 combines the original evaluations and what we know from reactor theory to go directly to the heart of the matter and explicitly conserve the physical observables that we are interested in, such as flux, reaction rates, and average cross sections.

This approach is one of the reasons that TART95 can run to convergence so much faster than other Monte Carlo codes, and it is all automatic; the user doesn't have to be an expert in variance reduction, or even understand in detail everything that has been said here about

the multi-band method. All the user has to do is by input tell TART95 to use the multi-band method (**sentl 20 1**), (**highly recommended**) and that's it.

Kinematics

Interpolation

TART95 is designed to use the Livermore ENDL neutron interaction data and neutron induced photon production data, as well as the Livermore EGDL photon interaction data. As such in order to be completely consistent with the Livermore ENDL and EGDL conventions to linearly interpolate between tabulated values, TART95 also linearly interpolates between tabulated values. When using any other source of data, e.g., ENDF/B-VI, it is first converted to linear interpolable form before it is processed for use by TART95.

For neutron interaction cross sections TART95 uses multi-group cross sections, so that no interpolation in energy is required. For photon interaction cross sections TART95 uses 176 tabulated energy points between 100 eV and 30 MeV, and linearly interpolates between tabulated values.

The main place that TART95 uses interpolation is in sampling energy and angular distributions after a collision has occurred. Starting from ALL of the incident neutron and photon energies in ENDL and EGDL where distributions are tabulated, the distribution at EACH incident energy is exactly normalized to unity and divided into equally probable bins for sampling. In principle the data used by TART95 can be divided into any number of equally probable bins. In practice a standard number of bins have been used for many years for each type of data. The number of bins used has been defined to insure that the uncertainty introduced by binning the data is small, or at least comparable, to the uncertainty in energy and angular distributions. Based on the uncertainty in energy and angular distributions 32 equally probable bins are used for most distributions. The exception is for fission spectra, that due to their importance are binned using 1024 equally probable bins.

Each distribution is defined at a series of incident neutron or photon energies, spanning the entire energy range for each process, e.g., for neutron elastic scattering angular distributions are defined over the entire energy range, whereas for neutron inelastic scattering from a specific level, angular distributions are defined from the threshold of the level up to the maximum energy. At each incident energy any probability distribution, p(X), is defined by a table of equally probable values of X, i.e., X_1, X_2, X_3,.....X_{Jmax+1}, where for J_{max} equally probable intervals we need J_{max} + 1 ends of the intervals to define the entire distribution.

To sample any distribution TART95 first uses the incident neutron or photon energy to define the energy interval to interpolate within. For example, if the elastic scattering angular distributions are tabulated at a series of energies, E_1, E_2, E_3,....E_n, TART95 first

determines that based on the incident neutron energy, E, this energy is in the interval between E_2 and E_3. TART95 next uses a random number, R_1, to randomly select a bin, J, between the first and maximum number of equally probable bins, J_{max},

$$J = J_{max} R_1 + 1$$

and a second random number, R_2, to linearly interpolate within the selected bin. Using the same selected bin, J, and random number, R_2, the linear interpolation within the selected bin is performed at both ends of the tabulated incident energy interval. For example, if the incident neutron energy, E, is between the energies E_2 and E_3 where the distributions are tabulated, TART95 defines interpolated results within bin, J, at both E_2 and E_3,

$$X_2 = X_{2,J} + R_2 (X_{2,J+1} - X_{2,J})$$

$$X_3 = X_{3,J} + R_2 (X_{3,J+1} - X_{3,J})$$

to define the interpolated values X_2 and X_3, at energies E_2 and E_3, respectively.

Note, this sampling method treats each distribution as a histogram within each equally probable bin; it does not assume that the probability distribution. p(X), is linearly interpolable, but rather that the integral of, p(X), is linearly interpolable, which is equivalent to assuming the probability distribution, p(X), is constant within each equally probable bin.

Finally TART95 linearly interpolates in incident energy, E, between the interpolated values X_2 and X_3 at energies E_2 and E_3, to define the final sampled value X,

$$X = X_2 + (E - E_2) (X_3 - X_2)/(E_3 - E_2)$$

In this example the sampled values, X, could be scattering cosines for tabulated angular distributions, or a secondary energy for tabulated neutron spectra.

In most cases only this simple method of interpolation is required to define the final state of the incident neutron or photon after a collision. For example, for elastic or inelastic scattering from a discrete level, sampling the scattering cosine uniquely defines the completely correlated secondary energies. In other cases the scattering cosine and secondary energy are treated as uncorrelated and each is sampled independently using the method described above.

However, in the case of completely correlated energy-angular distributions a second level of interpolation is required. For this type of data at each incident energy the distribution is represented first by a series of equally probable cosines, and at each equally probable cosine a normalized spectrum is defined by a series of equally probable secondary energies. Note, for simplicity of sampling the entire distribution integrated over energy and angle is not normalized to unity. Rather the distribution is normalized by integrating over

cosine to define equally probable scattering cosines. The secondary energy spectrum at each equally probable cosine is then independently normalized to unity for efficiency of sampling. Sampling this type of data involves first sampling a cosine using the method described above, and once a cosine has been sampled then sampling the secondary energy from the normalized spectrum at the previously sampled cosine.

The definition of how to normalize this type of distribution makes the sampling particularly simple, since in this case we can first sample a cosine by the method described above using a distribution that is normalized to unity when interpolated over cosine. For the sampled cosine interval we can then sample from the spectra that are also normalized to unity at each equally probable cosine. Final we can then interpolate in cosine to sample a secondary energy. For example, if again the incident energy, E, is between the energies E_2 and E_3 where the distribution is tabulated, we can sample the cosine using,

$J = J_{max} R_1 + 1$; J_{max} is the number of equally probable cosine bins

$$Cos_2 = Cos_{2,J} + R_2 (Cos_{2,J+1} - Cos_{2,J})$$

$$Cos_3 = Cos_{3,J} + R_2 (Cos_{3,J+1} - Cos_{3,J})$$

$$Cos = Cos_2 + (E - E_2) (Cos_3 - Cos_2)/(E_3 - E_2)$$

Since the secondary energy spectrum at each equally probable cosine is independently normalized we can next sample the spectra at Cos_2 and Cos_3,

$K = K_{max} R_3 + 1$; K_{max} is the number of equally probable secondary energy bins

$$E'_2 = E'_{2,K} + R_4 (E'_{2,K+1} - E'_{2,K})$$

$$E'_3 = E'_{3,K} + R_4 (E'_{3,K+1} - E'_{3,K})$$

Finally interpolate in cosine to the previously selected Cos, to define the sampled secondary energy, E'.

$$E' = E'_2 + (Cos - Cos_2) (E'_3 - E'_2)/(Cos_3 - Cos_2)$$

Neutron Interactions

For tracking neutrons TART95 primarily uses speed, V, rather than energy, E. This is because since TART95 is a time dependent code it needs the speed to define the time scale in which events are happening. In addition many of the kinematic relationships can be more efficiently expressed in terms of speed. Therefore in the following discussion the methods will be described in terms of sampling speeds and/or energies.

Elastic and Inelastic Level Scattering

In these cases the scattering angle in the center-of-mass system is completely correlated to the secondary energy of the neutron after collision. Therefore in these cases TART95 first samples the angular distribution. Based on the ENDL data the scattering angle is either sampled from an isotropic distribution, or from an equally probable binned anisotropic distribution, as described above under the section on interpolation, to define the center of mass scattering cosine, Cos. It then defines the laboratory secondary energy, E', or secondary speed, V', and scattering cosine using,

$$V' = V [B^2 + 2 B Cos + 1]^{1/2}/[A +1]$$

$$Cos_L = [1 + B Cos]/[B^2 + 2 B Cos + 1]^{1/2}$$

Cos = center-of-mass scattering cosine
Cos_L = laboratory scattering cosine
V = incident neutron speed
V' = secondary neutron speed
A = atomic weight of target nucleus
B = A (for elastic scattering)
= $A [1 - (A+1) E_L/(A V^2)]^{1/2}$ (for inelastic scattering)
E_L = inelastic level energy

Thermal Elastic Scattering

The above model of elastic scattering assumes that the target nuclei are stationary. In order to treat thermal scattering TART95 using a free gas model, which assumes that the target nuclei are distributed in an isotropic Maxwellian distribution in the lab frame of reference. In order to consistently use this model we must discuss both the treatment of cross sections (to properly define reaction rates and therefore distance to collision) and kinematics (to properly define the direction and secondary energy of a neutron after it has undergone an elastic collision).

In order to predict the correct reaction rates the neutron interaction cross sections have been Doppler broadened using the SIGMA1 method [36] to process the cross sections read by TART95 for use in calculations. The SIGMA1 method is consistent with the free gas model in general and does not require any assumption about the angular distribution of neutrons after collision; an additional assumption concerning the angular distribution will be introduced when we discuss kinematics below. The standard TART95 neutron interaction data file, TARTND, has been prepared at room temperature (293 Kelvin). Additional data files for use with TART95 can be prepared for any temperature above room temperature.

In order to predict the direction and energy of a neutron after it collides with a moving nucleus TART95 assumes that this will only occur at relatively low energies where the angular distribution for elastic scattering is isotropic in the center-of-mass system; the

assumption of isotropic scattering greatly simplifies the algorithm used. TART95 samples a target nucleus speed and direction from an isotropic (in the lab) Maxwellian; once these have been sampled it knows the relative speed and can therefore define the equations in the center-of-mass system. Since we assume isotropic scattering in the center-of-mass system the neutron direction after the collision is completely random and uncorrelated to its initial direction of motion. Therefore TART95 can randomly select new directions, and finally add in the center-of-mass motion to transform back to the lab system to define the final neutron direction and energy [see, 35]. The equations are similar to those described above for elastic scattering off a stationary target, but the actual algorithm used is greatly simplified since we need not first sample from an equally probable binned distribution; this is because we assume isotropic scattering in the center-of-mass system.

Warning - in order to consistently use this thermal scattering model it is important that the Doppler broadened cross sections and kinematic sampling both use exactly the same temperature for the medium through which the neutrons are transporting. For example, you will not obtain consistent results if you use cross sections that have been Doppler broadened to room temperature (293 Kelvin) in a problem in which your TART95 input parameters specify the temperature to be 2000 Kelvin. If you do this the reaction rate and distance to collision will be based on the 293 Kelvin cross sections and the thermal scattering kinematics will be based on the 2000 Kelvin temperature that you specified by input.

Multiple neutron emission

For (n,2n), (n,3n), etc., where multiple neutrons are emitted secondary direction and energy are treated as uncorrelated. In this case, based on the emitted neutron multiplicity [2 for (n,2n), 3 for (n,3n), etc.], each neutron is independently sampled from the given distributions, e.g., for (n,2n) no attempt is made to correlate the secondary energy or direction of the two emitted neutrons. Each emitted neutron will have its secondary energy sampled from an equally probable binned distribution as described above. Based on the data in TARTND, the direction of each neutron will either be sampled from an isotropic distribution or from an equally probable binned anisotropic angular distribution.

For fission, which is a special case of multiple neutron emission, TART95 will emit an integral number of secondary neutrons, i.e., 1, 2, 3, etc. based on the average number of secondary neutrons emitted per fission, (i.e., based on nu-bar), in a manner that will statistically reproduce the correct average number of neutrons per fission. As in the case of other multiple neutron emission processes, each emitted neutron will be independently sampled from equally probable binned fission spectra and either isotropic or binned equally probable anisotropic angular distributions. If we know the average number of neutrons emitted per fission, nu-bar, TART95 will select a random number, R1, and emit an integral number of fission neutrons,

I = nu-bar + R1

For example if nu-bar is 2.7, using this algorithm statistically 30 % of the time TART95 will emit 2 neutrons and 70 % it will emit 3 neutrons, to statistically re-produce the correct average of 2.7 neutrons.

Correlated (n,2n)

The user has the input option to specify that (n,2n) spectra should be sampled to correlate the energy, see **sentl 50**. If this sentinel is not set by input the emission of (n,2n) neutrons is as described above. When this sentinel is set the first of the two emitted neutrons is sampled as described above. Based on the selection of the first neutron energy, the second neutron energy is sampled from the complementary probability point in the binned energy spectrum. For example, if the energy distribution is in 32 equally probable bins and we use random numbers, R_1, to select a bin, and R_2 to interpolate within the bin, we can define the sampled energy of the first emitted neutron to be,

$$J = 32\,R_1 + 1$$

$$E'_2 = E'_{2,J} + R_2\,(E'_{2,J+1} - E'_{2,J})$$

$$E'_3 = E'_{3,J} + R_2\,(E'_{3,J+1} - E'_{2,J})$$

$$E' = E'_2 + (E - E_2)\,(E'_3 - E'_2)/(E_3 - E_2)$$

The second neutron is then emitted by sampling from the complementary probability point in the probability distribution which is in bin,

$$J' = 33 - J$$

at the point,

$$R'_2 = 1 - R_2$$

The equations used are the same as those used above for the first neutron, with J and R_2 and replaced by J' and R'_2.

Compared to uncorrelated (n,2n) sampling, this method will tend to speed sampling convergence toward the correct average emitted neutron energy.

Whether or not this option is selected the direction of the two emitted neutrons will still be uncorrelated; this option only tries to correlate emitted energies, not directions.

The Cluster Model

The Cluster Model is another model used to describe correlated (n,2n). This model assumes that the first emitted neutron is emitted from a discrete inelastic level of the

compound nucleus. Therefore the treatment of the first emitted neutron is exactly the same as for the case of inelastic scattering, described above. It is then assumes that the second emitted neutron moves in the same direction and at the same speed as the recoil nucleus.

Currently this model is only used to model (n,2n) for neutrons incident on deuterium, where the first neutron is emitted from the 2.23 MeV level of the compound nucleus, leaving a neutron and proton to recoil at the same speed and in the same direction (at least initially; they will eventually separate since the distance to the next collision will differ for neutrons and protons).

As described above for inelastic scattering, for the first emitted neutron the center-of-mass scattering cosine, Cos, is first sampled, and the laboratory speed and scattering cosine are defined using,

$$S = [B^2 + 2\ B\ Cos\ +\ 1]^{1/2}$$

$$V' = V\ S/[A+1]$$

$$Cos_L = [1 + B\ Cos]/S$$

Cos = center-of-mass scattering cosine
Cos_L = laboratory scattering cosine
V = incident neutron speed
V' = secondary neutron speed
A = atomic weight of target nucleus
B = $A\ [1 - (A+1)\ E_L/(A\ V^2)]^{1/2}$
E_L = inelastic level energy

The recoil nucleus speed and direction are defined by,

$$S = [B^2/A^2 - 2\ B\ Cos/A\ +\ 1]^{1/2}$$

$$V'_R = V\ S/[A+1]$$

$$Cos_R = [1 - B\ Cos/A]/S$$

This is the speed and scattering angle assigned to the second emitted neutron.

Photon Interactions

Starting from the Livermore photon interaction data file, EGDL, the photon interaction cross sections have been processed into a fixed energy grid form using the same 176 energy points between 100 eV and 30 MeV, for all processes and all elements; see the appendix for a table of the 176 energy points. TART95 linearly interpolates between tabulated value to define photon cross on a continuous basis to any given photon energy.

Coherent Scattering

By definition the photon does not change energy during coherent scattering. The scattering angle for coherent scattering is defined by the product of Rayleigh scattering and the coherent form factor,

$R(Cos) = C(Z)\,[Cos^2 + 1]$ = Rayleigh scattering

$f(Cos) = R(Cos)\,FF^2$

C(Z) = is an element (Z) dependent constant
FF = the coherent form factor
f(Cos) = the coherent scattering angular distribution

The details of how TART95 samples this distribution are described in the report of Brown, McIntosh and Terrall [15]. Basically for sampling by TART95 the distribution is scaled to account for Z (atomic number) dependence and integrated into 64 equally probable bins. The result is one simple binned integral that is universally applied to all elements.

Incoherent Scattering

The scattering angle and secondary energy of the photon are defined by the product of the Klein-Nishina formula and the incoherent scattering function,

$$KN(E, Cos) = \frac{[Cos^2 + 1][1 + A\,x] + [Ax]^2}{[1 + A\,x]^3}$$ = Klein-Nishina formula

A = photon energy in electron mass units (0.511 MeV)
x = 1 - Cos
A' = A/[1 + Ax] = secondary photon energy

$f(Cos) = KN(E, Cos)\,SF$

SF = the incoherent scattering function
f(Cos) = the incoherent scattering angular distribution

The details of how TART95 samples this distribution are described in the report of Brown, McIntosh and Terrall [15]. Basically, for sampling by TART95 the distribution is scaled to account for Z (atomic number) dependence and at 26 incident photon energies it is integrated into 200 equally probable bins. The result is binned integrals at 26 incident energies that is universally applied to all elements.

Pair Production

For each pair production event it is assumed that the electron and positron will slow down and stop near the point where the pair production event occurred. It is assumes that the positron will stop and annihilate, producing two 0.511 MeV photons at the point where the pair production event occurred. Since we assume the positron has stopped, the direction of the two 0.511 MeV photons is completely random. The direction of one 0.511 MeV photon is randomly selected and the second photon is then directed in the opposite direction, to conserve momentum.

Photoelectric

Unless the track fluorescence option (**sentl 25**) is turned on by user input, each photoelectric event terminates the history and all of the photons energy is deposited.

Fluorescence

If fluorescence x-ray tracking is turned on by user input, TART95 considers K and L shell fluorescence. It assumes that above the K edge the ratio of cross sections for the shells remains constant. Similarly above the L_3 edge it assumes the ratio of cross sections is constant. Using this assumption for each photoelectric event where the incident photons energy is greater than the K edge energy we can statistically define which shell was ionized, i.e., has a vacancy. Similarly for energies below the K edge, but above the L_3 edge, it can statistically define which shell was ionized.

Once it has been statistically determined which shell has a vacancy we can use the probability of fluorescence for that shell to statistically determine whether or not fluorescence is emitted. If fluorescence is emitted, we can use the probability of each individual transition to statistically define which transition occurs. We then emit a photon with an energy equal to the difference in binding energies for the two subshells involved in the transition.

In the case where the first, primary, transition described above is a K - L transition (a radiative transition where an electron moves from the L shell to fill a hole in the K shell) the result will be a vacancy in the L shell. In this case we will repeat the procedure described above to statistically emit a second fluorescence x-ray; what is referred to as a secondary transition.

For each element we have the energy of the photoelectric edges, i.e., the electron binding energies,

EK - energy of K edge
EL1 - energy of L_1 edge
EL2 - energy of L_2 edge
EL3 - energy of L_3 edge

EM1 - energy of M_1 edge
EM2 - energy of M_2 edge
EM3 - energy of M_3 edge
EM4 - energy of M_4 edge
EM5 - energy of M_5 edge

Above the K edge we have,

VKK - probability of K vacancy
VKL - probability of L vacancy
VKM - probability of M vacancy
VKO - probability of Other vacancy
FKK - probability of K shell fluorescence
FKL - probability of L shell fluorescence

Since a vacancy must occur in some shell the sum of the vacancy probabilities is one.

The following primary transitions are considered

K - L_3 (K alpha 1)
K - L_2 (K alpha 2)
K - M_3 (K beta)
L_3 - M_5
L_2 - M_4

for which we have,

PKL3 - probability of K - L_3 transition
PKL2 - probability of K - L_2 transition
PKM3 - probability of K - M_3 transition
PL2M4 - probability of L2 - M4 transition (assumed constant 0.371)
PL3M5 - probability of L3 - M5 transition (assumed constant 0.629)

These probabilities are normalized such that the sum of the probability of K transitions is one, and the sum of the L transitions is one.

If a K - L transition occurs the result will be a secondary vacancy in the L shell, and the following secondary transitions are considered,

L_3 - M_5
L_2 - M_4

The sampling procedure is as follows,

1) Statistically sample a vacancy in K, L, M or Other shell

2) If the vacancy is in the K or L shell, statistically sample the probability of fluorescence
3) If fluorescence occurs, statistically select the transition,

K - L_3	- emit a photon with energy EK - EL3
K - L_2	- emit a photon with energy EK - EL2
K - M_3	- emit a photon with energy EK - EM3
L_3 - M_5	- emit a photon with energy EL3 - EM5
L_2 - M_4	- emit a photon with energy EL2 - EM4

4) If fluorescence was emitted due to a K - L_3 or K - L_2 transition,
statistically sample the probability of L shell fluorescence
5) If L shell fluorescence occurs, statistically select the transition,

L_3 - M_5	- emit a photon with energy EL3 - EM5
L_2 - M_4	- emit a photon with energy EL2 - EM4

6) Otherwise, there is no fluorescence

Below the K edge, but above the L edge we have,

VLL - probability of L vacancy
VLM - probability of M vacancy
VLO - probability of Other vacancy
FLL - probability of L shell fluorescence
FLM - probability of M shell fluorescence

The following primary transitions are considered

L_3 - M_5
L_2 - M_4

for which we have,

PL2M4 - probability of L2 - M4 transition (assumed constant 0.371)
PL3M5 - probability of L3 - M5 transition (assumed constant 0.629)

These probabilities are normalized such that the sum of the probability of L transitions is one.

In this case no secondary transitions are considered, i.e., M shell fluorescence is ignored.

The sampling procedure is as follows,

1) Statistically sample a vacancy in L, M or Other shell
2) If the vacancy is in the L shell, statistically sample the probability of

fluorescence
3) If fluorescence occurs, statistically select the transition,

L_3 - M_5 - emit a photon with energy EL3 - EM5
L_2 - M_4 - emit a photon with energy EL2 - EM4

4) Otherwise, there is no fluorescence

Below the L_3 edge fluorescence is ignored.

Neutron Induced Photon Production

For any given material there can be photon production data for any number of neutron reactions. The data can be directly associated with an individual reaction, e.g., the emission of a specific photon line following an inelastic scattering from a specific level. Alternatively it can be associated with a general emission spectrum that experimentally and theoretically cannot be directly associated with an individual neutron interaction, e.g., emission from a continuum of inelastic states, or a cascade of photons from a number of competing processes.

For any given material there can be a set of photon production data for any number of neutron reactions. Each set of photon production data has a photon production cross section associated with it. Following each neutron interaction (regardless of what neutron interaction was statistically sampled), the probability and number of photons produced (the photon multiplicity), is defined as the ratio of the photon production cross section for each set of photon production data to the total neutron interaction cross section. Following each neutron interaction TART95 samples every single set of photon production data and allows all to statistically emit photons. Let me again state that this procedure is as close as possible to what is experimentally measured, reported and is best known. For example, even following an elastic collision TART95 will allow statistical emission of photons. This procedure statistically works because the ENDL data has been designed to insure an exact energy balance to on average conserve the division of energy between neutrons after each reaction and the photons produced per reaction.

TART95 always emits an integer number of photons. To decide how many photons to emit TART95 uses the total neutron interaction cross section, sig_{tot}, selects a random number, R1, and starts with the photon production cross section for the first set of data, $sigpp_1$, to define,

$R_1 = sigpp_1/sig_{tot} + R1$

If R_1 is greater than or equal to unity emit a photon from this set of data (as described below), decrement R_1 by one and continue emitting photons from this set of data and decrementing R_1 until R_1 is less than unity. When R_1 becomes less than unity we proceed to the next set of photon production data and use its cross section, $sigpp_2$, to define,

R_1 = sigpp$_2$/sig$_{tot}$ + R1

Again we emit photons from this set and decrement R_1 until R_1 is less than unity. This cycle continues through ALL of the sets of photon production data, allowing each to statistically emit photons

Note, in this algorithm we only select one initial random number, R_1, and continue to use the integer remainder of R_1 for each successive set of photon production data. Therefore if we sum over all sets of data statistically the integer number of photons produced is,

N = sum[k=1 to m] sigpp$_m$/sig$_{tot}$ + R_1, m = the number of sets of data

Once we have used the photon production cross section for a given set of data to decide to emit a photon, we must next sample the distribution of photon energies and directions for the set; how this is done is described below.

There are four different representations of neutron induced photon production data energy and direction distributions used by TART95,

1) Energy lines, isotropic
2) Energy lines, anisotropic
3) Energy Continuum, isotropic
4) Energy Continuum, anisotropic

In all cases photon energy and direction are uncorrelated. Therefore sampling of the angular distribution is performed in exactly the manner described above under the section on interpolation, and need not be discussed again here. The same is true for energy continuum. Both angular and energy continuum are binned in 32 equally probable bins and sampled exactly as described above.

The energy lines are represented as a normalized integral probability distribution, which allows each line to be sampled according to the weight it contributes to the normalized integral, and emission is exactly at the energy of each line.

WARNING - Repeating the warning given above - The ENDL neutron interaction and neutron induced photon production cross sections have been designed to be completely consistent when used in combination, as have other neutron data libraries. But the user MUST be aware that to perform consistent coupled neutron-photon transport calculations if you use any alternative data sets you MUST consistently use both neutron interaction and photon production data from the same alternative set of data. For example, for coupled neutron-photon calculations you SHOULD NOT use ENDF/B-VI neutron interaction data and ENDL neutron induced photon production data.